

S. N. 10/603474

LANGEL 10/603474 1/24/05 Page 1

=> FILE HCAPL

FILE 'HCAPLUS' ENTERED AT 15:31:10 ON 24 JAN 2005

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FILE COVERS 1907 - 24 Jan 2005 VOL 142 ISS 5

FILE LAST UPDATED: 23 Jan 2005 (20050123/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D QUE L31

L4 1786 SEA FILE=REGISTRY ABB=ON (M(L)H(L)N)/ELS(L)3/ELC.SUB
L5 4217 SEA FILE=REGISTRY ABB=ON (M(L)H)/ELS(L)2/ELC.SUB
L6 1 SEA FILE=REGISTRY ABB=ON HYDROGEN/CN
L8 23856 SEA FILE=HCAPLUS ABB=ON L5
L10 92 SEA FILE=REGISTRY ABB=ON L4 AND IMIDE
L11 171 SEA FILE=HCAPLUS ABB=ON L10
L12 1694 SEA FILE=REGISTRY ABB=ON L4 NOT L11
L13 221 SEA FILE=REGISTRY ABB=ON L4 AND IMID?
L14 1565 SEA FILE=REGISTRY ABB=ON L12 NOT L13
L15 356 SEA FILE=REGISTRY ABB=ON L14 AND AMID?
L16 219 SEA FILE=HCAPLUS ABB=ON L13
L17 2271 SEA FILE=HCAPLUS ABB=ON L15
L18 83 SEA FILE=HCAPLUS ABB=ON (L11 OR L16) AND L17
L19 18 SEA FILE=HCAPLUS ABB=ON L18 AND L8
L26 15 SEA FILE=HCAPLUS ABB=ON L19 AND (L6 OR HYDROGEN OR H2)
L27 9472 SEA FILE=HCAPLUS ABB=ON (L6 OR H2 OR HYDROGEN) (4A)STOR?
L28 5 SEA FILE=HCAPLUS ABB=ON L26 AND L27
L29 119841 SEA FILE=HCAPLUS ABB=ON (L6 OR H2 OR HYDROGEN) (L)PROC/RL
L30 6 SEA FILE=HCAPLUS ABB=ON L26 AND L29
L31 7 SEA FILE=HCAPLUS ABB=ON L28 OR L30

=> FILE WPIX

FILE 'WPIX' ENTERED AT 15:31:38 ON 24 JAN 2005

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FILE LAST UPDATED: 17 JAN 2005 <20050117/UP>

MOST RECENT DERWENT UPDATE: 200504 <200504/DW>

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KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

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 PLEASE CHECK:
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 FOR DETAILS. <<<

=> D QUE L49

L6 1 SEA FILE=REGISTRY ABB=ON HYDROGEN/CN
 L33 5292 SEA FILE=WPIX ABB=ON (L6 OR H2 OR HYDROGEN) (4A)STOR?
 L34 4 SEA FILE=WPIX ABB=ON L33 AND ?AMID? AND ?IMID? AND ?HYDRIDE?
 L47 8 SEA FILE=WPIX ABB=ON L33 AND ?AMID? AND ?IMID?
 L48 8 SEA FILE=WPIX ABB=ON L34 OR L47
 L49 2 SEA FILE=WPIX ABB=ON L48 AND C01B?/IC

=> D QUE L48

L6 1 SEA FILE=REGISTRY ABB=ON HYDROGEN/CN
 L33 5292 SEA FILE=WPIX ABB=ON (L6 OR H2 OR HYDROGEN) (4A)STOR?
 L34 4 SEA FILE=WPIX ABB=ON L33 AND ?AMID? AND ?IMID? AND ?HYDRIDE?
 L47 8 SEA FILE=WPIX ABB=ON L33 AND ?AMID? AND ?IMID?
 L48 8 SEA FILE=WPIX ABB=ON L34 OR L47

=> FILE JAPIO

FILE 'JAPIO' ENTERED AT 15:32:16 ON 24 JAN 2005
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FILE LAST UPDATED: 4 JAN 2005 <20050104/UP>
 FILE COVERS APR 1973 TO SEPTEMBER 30, 2004

<<< GRAPHIC IMAGES AVAILABLE >>>

=> D QUE L46

L6 1 SEA FILE=REGISTRY ABB=ON HYDROGEN/CN
 L33 5292 SEA FILE=WPIX ABB=ON (L6 OR H2 OR HYDROGEN) (4A)STOR?
 L35 0 SEA FILE=JAPIO ABB=ON L33 AND ?AMID? AND ?IMID? AND ?HYDRIDE?
 L45 0 SEA FILE=JAPIO ABB=ON L33 AND ?AMID? AND ?IMID?
 L46 0 SEA FILE=JAPIO ABB=ON L35 OR L45

=> FILE COMPEN

FILE 'COMPENDEX' ENTERED AT 15:32:29 ON 24 JAN 2005
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FILE LAST UPDATED: 24 JAN 2005 <20050124/UP>
FILE COVERS 1970 TO DATE.

<<< SIMULTANEOUS LEFT AND RIGHT TRUNCATION AVAILABLE IN
THE BASIC INDEX >>>

=> D QUE L44

L6 1 SEA FILE=REGISTRY ABB=ON HYDROGEN/CN
L33 5292 SEA FILE=WPIX ABB=ON (L6 OR H2 OR HYDROGEN) (4A)STOR?
L36 3 SEA FILE=COMPENDEX ABB=ON L33 AND ?AMID? AND ?IMID? AND
?HYDRIDE?
L43 4 SEA FILE=COMPENDEX ABB=ON L33 AND ?AMID? AND ?IMID?
L44 4 SEA FILE=COMPENDEX ABB=ON L43 OR L36

=> FILE INSPEC

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FILE COVERS 1969 TO DATE.

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THE BASIC INDEX >>>

=> D QUE L42

L6 1 SEA FILE=REGISTRY ABB=ON HYDROGEN/CN
L33 5292 SEA FILE=WPIX ABB=ON (L6 OR H2 OR HYDROGEN) (4A)STOR?
L37 1 SEA FILE=INSPEC ABB=ON L33 AND ?AMID? AND ?IMID? AND ?HYDRIDE?
L40 1 SEA FILE=INSPEC ABB=ON L33 AND ?AMID? AND ?IMID?
L42 1 SEA FILE=INSPEC ABB=ON L37 OR L40

=> FILE JICST

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FILE COVERS 1985 TO 17 JAN 2005 (20050117/ED)

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TERM (/CT) THESAURUS RELOAD.

=> D QUE L39

L6 1 SEA FILE=REGISTRY ABB=ON HYDROGEN/CN
L33 5292 SEA FILE=WPIX ABB=ON (L6 OR H2 OR HYDROGEN) (4A)STOR?
L39 1 SEA FILE=JICST-EPLUS ABB=ON L33 AND ?AMID? AND ?IMID?

=> DUP REM L31 L48 L44 L42 L39

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PROCESSING COMPLETED FOR L48
PROCESSING COMPLETED FOR L44
PROCESSING COMPLETED FOR L42
PROCESSING COMPLETED FOR L39
L50 19 DUP REM L31 L48 L44 L42 L39 (2 DUPLICATES REMOVED)

=> D L50 ALL 1-19

L50 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:976 HCAPLUS
DN 142:77674
ED Entered STN: 31 Dec 2004
TI Imide/amide **hydrogen storage** system
IN Meisner, Gregory P.; Pinkerton, Frederick E.; Meyer, Martin S.; Balogh, Michael P.; Kundrat, Matthew D.
PA USA
SO U.S. Pat. Appl. Publ., 8 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM C01B021-087
NCL 423658200; 423413000
CC 52-3 (Electrochemical, Radiational, and Thermal Energy Technology)
Section cross-reference(s): 49
FAN.CNT 1

applicant

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2004265226	A1	20041230	US <u>2003-603474</u>	20030625
US 2004265222	A1	20041230	US 2004-824876	20040415
WO 2005005310	A2	20050120	WO 2004-US16529	20040525
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRAI US 2003-603474	A3	20030625		

US 2004-824876 A 20040415

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2004265226	ICM	C01B021-087
	NCL	423658200; 423413000

AB **Hydrogen** is **stored** by contacting gaseous **hydrogen** with an imide $\text{Mc}(\text{NH})\text{-}2\text{c}/2$ forming an amide $\text{Md}(\text{NH}_2)\text{d-}1$ and a hydride. Preferably, Li_2NH reacts with **H2** to LiNH_2 and LiH or MgNH reacts with **H2** to $\text{Mg}(\text{NH}_2)_2$ and MgH_2 . The **hydrogen** can be released by ball milling the amide and the hydride under an inert gas atmospheric and heating.

ST metal imide amide hydride **hydrogen storage** system

IT Ball milling
(imide/amide **hydrogen storage** system)

IT **7693-27-8**, Magnesium hydride **7803-54-5**, Magnesium amide ($\text{Mg}(\text{NH}_2)_2$)
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); FORM (Formation, nonpreparative); **PROC (Process)**
(imide/amide **hydrogen storage** system)

IT **7580-67-8**, Lithium hydride **7782-89-0**, Lithium amide **26134-62-3**, Lithium nitride **26134-80-5**, Magnesium imide
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); **PROC (Process)**; RACT (Reactant or reagent)
(imide/amide **hydrogen storage** system)

IT **12135-01-2P**, Lithium imide
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **PROC (Process)**; RACT (Reactant or reagent)
(imide/amide **hydrogen storage** system)

IT **1333-74-0**, **Hydrogen**, processes
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); **PROC (Process)**
(**storage**; imide/amide **hydrogen storage** system)

L50 ANSWER 2 OF 19 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN

AN 2004-304040 [28] WPIX

DNN N2004-242109 DNC C2004-115560

TI Composite pressure container or tubular body for compressed natural gas tanks, comprises prepreg tow winding obtained by contacting fiber(s) with uncured thermosetting resin, winding coated fiber around outer shell, and curing resin.

DC A17 A21 A25 A32 A92 P42 P73 Q65 Q69

IN SANTOU, I; SANTO, I

PA (MITR) MITSUBISHI RAYON CO LTD; (SANT-I) SANTO I

CYC 35

PI	US 2004052997	A1	20040318	(200428)*	11	B32B001-08
	CA 2440806	A1	20040317	(200428)	EN	F17C001-06
	EP 1400342	A2	20040324	(200428)	EN	B29C070-50
		R:	AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV MC MK NL PT RO SE SI SK TR			
	JP 2004106552	A	20040408	(200428)	21	B29C070-16
	CN 1490150	A	20040421	(200446)		B29C063-06
ADT	US 2004052997	A1	US 2002-244749	20020917;	CA 2440806	A1 CA 2003-2440806
			20030912;	EP 1400342	A2 EP 2003-20502	20030915;
			JP 2004106552	A	JP 2003-325227	20030917;
			CN 1490150	A	CN 2003-156994	20030917

PRAI US 2002-244749 20020917

IC ICM B29C063-06; B29C070-16; B29C070-50; B32B001-08; F17C001-06
ICS B05D003-02; B29B015-12; B29C053-56; B29C070-06; B29C070-30;
B29C070-68; B65H081-00; C08J005-04; C08J005-24; D06M015-55;
F16J012-00; F17C001-16

AB US2004052997 A UPAB: 20040429

NOVELTY - A composite pressure container or tubular body, comprises a prepreg tow winding obtained by contacting fiber(s) with an uncured thermosetting resin, to form a coated fiber; winding the coated fiber around an outer shell, form, liner, or mandrel; and curing the resin. The uncured thermosetting resin comprises least one surface-active oligomer or polymer.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for:

(a) a process for producing a prepreg tow and/or a prepreg, comprising contacting reinforcing fiber(s) with a thermosetting resin, and a solution or an aqueous emulsion comprising water, to form a coated fiber; and vaporizing the water from the coated fiber;

(b) a prepreg or prepreg tow, comprising fiber(s), thermosetting resin(s), and at least one surface active oligomer or polymer;

(c) a reinforced fiber, comprising a fiber, thermosetting resin(s), and at least one surface active oligomer or polymer; and

(d) a pressure container or tubular body, comprising the reinforced fiber as above in contact with an inner shell or liner.

USE - Useful for applications, i.e. compressed natural gas tanks; breather oxygen tanks for, e.g. firefighters; **hydrogen storage** tanks for, e.g. fuel cells; offshore pipes; and flywheel rotors.

ADVANTAGE - The inventive composite pressure container or tubular body has prepreg tow in which the fiber strength translation of a hoop fiber is improved, and that can be produced in an ecologically friendly manner.

DESCRIPTION OF DRAWING(S) - The figure shows a schematic view of a process for producing a prepreg tow.

Creel 1

Resin addition device 2

Impregnation roller 3

Resin feed pipe 4

Resin tank 5

Oven 6

Winder 7

Dwg.1/1

FS CPI GMPI

FA AB; GI

MC CPI: A11-B09A1; A11-C02D; A12-P05; A12-S08D

L50 ANSWER 3 OF 19 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN

AN 2004-350601 [33] WPIX

DNC C2004-133511

TI Graft copolymer for resin composition, is obtained by reacting functional group-containing polyphenylene ether and specific amino group-containing hydrogenated polymer and/or amino group-containing polymer.

DC A18 A28 A84 A85 A95

IN AKIYAMA, Y; SAKATA, M; YAMAMOTO, G

PA (ASAHI) ASAHI KASEI KK

CYC 2

PI JP 2004059742 A 20040226 (200433)* 27 C08G081-02

DE 10334049 A1 20040304 (200433) C08L051-06

ADT JP 2004059742 A JP 2002-220188 20020729; DE 10334049 A1 DE 2003-10334049 20030725

PRAI JP 2002-220188 20020729

IC ICM C08G081-02; C08L051-06

ICS C08L023-02; C08L053-00; C08L071-12; C08L101-00

AB JP2004059742 A UPAB: 20040525

NOVELTY - A graft copolymer is obtained by reacting functional group-containing polyphenylene ether (in weight parts (wt.pts)) (99-1) and amino group-containing hydrogenated polymer (II) and/or amino group-containing polymer (1-99). The polymer (II) is obtained by reacting active terminal lithium ion group of vinyl aromatic compound-conjugated diene compound block copolymer chain with ring compound (1 or 2).

DETAILED DESCRIPTION - A graft copolymer is obtained by reacting functional group-containing polyphenylene ether (99-1) and amino group-containing hydrogenated polymer (II) and/or amino group-containing polymer (1-99). The polymer (II) is obtained by reacting active terminal lithium ion group of vinyl aromatic compound-conjugated diene compound block copolymer chain with ring compound of formula (1 or 2). The polyphenylene ether has acid ~~anhydride~~ group, epoxy group or carboxyl group. The block copolymer containing active terminal lithium ion group is obtained using organic lithium compound as polymerization initiator in hydrocarbon solvent.

R1,R2 = 1-4C alkyl group or alkoxy group;

Y = oxygen atom or sulfur atom;

n = 2-4;

R1 in formula (2) = 1-6C alkyl group, cycloalkyl group or alkoxy group; and

n in formula (2) = 3-4.

Hydrogen atom(s) of the polymethylene chain in formulae (1,2) is optionally substituted by 1-6C alkyl group.

An INDEPENDENT CLAIM is included for resin composition which contains 1-99 wt.pts of the graft copolymer and 99-1 wt.pts of thermoplastic resins.

USE - For resin composition (claimed) used as molding material, for external covering, motor vehicle component such as bumper, door panel, fender, emblem, engine hood, wheel cap, roof, interior component such as instrument panel and console box, for interior and exterior cladding component of electric equipment such as chassis, disk player, computer and its peripheral device, electronic office equipment, television, video, cabinet, refrigerator, DVDROM, DVDROM, CD, MP3, DVD-R, DVD-RW, CDROM, MD and CDR. The resin composition is also used for electrode and electrolyte liquid of lead **storage** battery, nickel-**hydrogen** battery and lithium ion battery.

ADVANTAGE - The graft copolymer provides resin composition with favorable miscibility, improved cold shock strength, heat-resistant property, workability and weld tensile strength.

Dwg.0/0

FS CPI

FA AB; GI

MC CPI: A10-E01

L50 ANSWER 4 OF 19 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN

AN 2004-489888 [47] WPIX

DNN N2004-386399 DNC C2004-182479

TI Dispensing apparatus for dispensing odorant to hydrogen gas, e.g. for fuel cell, includes **hydrogen storage** material disposed in interior volume of first or second container.

DC A85 E36 L03 S02 X16

IN PEZ, G P; PURI, P S

PA (AIRP) AIR PROD & CHEM INC; (PEZG-I) PEZ G P; (PURI-I) PURI P S

CYC 33

PI EP 1431735 A2 20040623 (200447)* EN 9 G01M003-20
 R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV
 MC MK NL PT RO SE SI SK TR
 CA 2452466 A1 20040616 (200447) EN G01M003-20
 US 2004126889 A1 20040701 (200447) G01N031-00

ADT EP 1431735 A2 EP 2003-28744 20031212; CA 2452466 A1 CA 2003-2452466
 20031209; US 2004126889 A1 US 2002-321326 20021216

PRAI US 2002-321326 20021216

IC ICM G01M003-20; G01N031-00

ICS G01M003-22

AB EP 1431735 A UPAB: 20040723

NOVELTY - A dispensing apparatus comprises container(s) having an interior volume, odorant material(s) disposed in the interior volume of a first container, and **hydrogen storage** material(s) disposed in the interior volume of the first container or interior volume of a second container. The odorant material has detectable odor(s).

DETAILED DESCRIPTION - An INDEPENDENT CLAIM is also included for a method for dispensing an odorant to a hydrogen gas comprising providing container(s) having an interior volume, odorant material(s) sorbed on a sorbent (11) and disposed in the interior volume of a first container, **hydrogen storage** material(s) (12) disposed in the interior volume of the first or second container; and applying a form of energy to the odorant material and to the **hydrogen storage** material and/or partially depressurizing the container(s) to release the **hydrogen** gas from the **hydrogen storage** material and the odorant material from the sorbent.

USE - For dispensing odorant to hydrogen gas (claimed) e.g. for a fuel cell.

ADVANTAGE - The inventive apparatus is capable of maintaining and dispensing uniform quantity of odorant at all time. It maintains constant concentration of the odorant throughout the supply of the gas.

DESCRIPTION OF DRAWING(S) - The figure is a simplified, cross-sectional view of a vessel containing odorant sorbent and **hydrogen storage** materials.

Vessel 10

Sorbent 11

Hydrogen storage material 12

Outlet 15

Dwg.1/3

FS CPI EPI

FA AB; GI; DCN

MC CPI: A12-E06; E10-C04F; E10-C04G2A; E10-C04L1; E10-G02H2E; E11-S; E31-A02;
 L03-E04

EPI: S02-J06A5; X16-C

L50 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 1

AN 2004:363485 HCAPLUS

DN 140:381348

ED Entered STN: 05 May 2004

TI Mechanism of Novel Reaction from LiNH₂ and LiH to Li₂NH and H₂
 as a Promising **Hydrogen Storage** System

AU Ichikawa, Takayuki; Hanada, Nobuko; Isobe, Shigehito; Leng, Haiyan; Fujii, Hironobu

CS Natural Science Center for Basic Research and Development, Hiroshima University, Higashi-Hiroshima, 739-8526, Japan

SO Journal of Physical Chemistry B (2004), 108(23), 7887-7892

CODEN: JPCBFK; ISSN: 1520-6106

PB American Chemical Society

DT Journal

LA English
 CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
 Section cross-reference(s): 52, 66
 AB The mechanism of the **hydrogen** desorption (HD) reaction from the 1:1 mixture of lithium amide (LiNH₂) and lithium hydride (LiH) to lithium imide (Li₂NH) and **hydrogen** (H₂) has been proposed on the basis of our exptl. results in this paper. The proposed model is constituted by 2 kinds of elementary reactions: the one is that 2LiNH₂ decomp. to Li₂NH and ammonia (NH₃), the other is that the emitted NH₃ reacts with LiH and transforms into LiNH₂ and H₂. Since the former and the latter reactions are, resp., endothermic and exothermic, the HD reaction corresponding to the latter reaction occurs as soon as LiNH₂ has decomposed into Li₂NH and NH₃. Therefore, the HD reaction can be understood by the following processes: at the first step, LiNH₂ decomp. into Li₂NH/2 + NH₃/2, and then the emitted NH₃/2 quickly reacts with LiH/2, transforming into LiNH₂/2 + H₂/2; at the second one, the produced LiNH₂/2 decomp. to Li₂NH/4 + NH₃/4, and then NH₃/4 + LiH/4 transform to LiNH₂/4 + H₂/4, and such successive steps continue until LiNH₂ and LiH completely transform into Li₂NH and H₂, even at low temps., by the catalytic effect of TiCl₃.
 ST mechanism reaction lithium amide hydride **hydrogen storage** system; imide lithium formation **hydrogen storage** system; titanium chloride catalyst mechanism reaction lithium amide hydride
 IT Catalysts
 Desorption
 Reaction mechanism
 (mechanism of reaction from LiNH₂ and LiH to Li₂NH and H₂ as promising **hydrogen storage** system)
 IT 7705-07-9, Titanium trichloride, uses
 RL: CAT (Catalyst use); USES (Uses)
 (mechanism of reaction from LiNH₂ and LiH to Li₂NH and H₂ as promising **hydrogen storage** system)
 IT 1333-74-0, **Hydrogen**, properties 12135-01-2,
 Lithium imide
 RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); **PROC (Process)**
 (mechanism of reaction from LiNH₂ and LiH to Li₂NH and H₂ as promising **hydrogen storage** system)
 IT 7580-67-8, Lithium hydride 7782-89-0, Lithium amide
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); **PROC (Process)**; RACT (Reactant or reagent)
 (mechanism of reaction from LiNH₂ and LiH to Li₂NH and H₂ as promising **hydrogen storage** system)
 RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE
 (1) Balema, V; J Alloys Compd 2000, V313, P69 HCAPLUS
 (2) Balema, V; J Alloys Compd 2001, V329, P108 HCAPLUS
 (3) Bogdanovic, B; J Alloys Compd 1997, V253, P1
 (4) Bogdanovic, B; J Alloys Compd 2000, V302, P36 HCAPLUS
 (5) Bogdanovic, B; MRS Bull 2002, September, P712
 (6) Chase, M; J Phys Chem Ref Data, Monograph 1998, V9, P1
 (7) Chen, P; J Phys Chem B 2003, V107, P10967 HCAPLUS
 (8) Chen, P; Nature 2002, V420, P302 HCAPLUS
 (9) Claudy, P; Mater Res Bull 1982, V17, P1499 HCAPLUS
 (10) Dafert, F; Monatsh Chem 1910, V31, P981
 (11) Gross, K; J Alloys Compd 2002, V330-332, P683 HCAPLUS

- (12) Hu, Y; Ind Eng Chem Res 2003, V42, P5135 HCAPLUS
- (13) Hu, Y; J Phys Chem A 2003, V107, P9737 HCAPLUS
- (14) Ichikawa, T; J Alloys Compd 2004, V365, P271 HCAPLUS
- (15) Isobe, S; In preparation
- (16) Jensen, C; Appl Phys A 2001, V72, P213 HCAPLUS
- (17) Jensen, C; Int J Hydrogen Energy 1999, V24, P461 HCAPLUS
- (18) Nakamori, Y; J Alloys Compd 2004, V370, P271 HCAPLUS
- (19) Ogita, N; Private communication
- (20) Ruff, O; Chem Ber 1911, V44, P502 HCAPLUS
- (21) Sandrock, G; J Alloys Compd 2002, V339, P299 HCAPLUS
- (22) Zaluski, L; J Alloys Compd 1999, V290, P71 HCAPLUS
- (23) Zidan, R; J Alloys Compd 1999, V285, P119 HCAPLUS

L50 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:807514 HCAPLUS

DN 141:352677

ED Entered STN: 04 Oct 2004

TI **Hydrogen storage** of metal nitride by a mechanochemical reaction

AU Kojima, Yoshitsugu; Kawai, Yasuaki

CS Toyota Central R&D Labs., Inc., Aichi, 480-1192, Japan

SO Chemical Communications (Cambridge, United Kingdom) (2004), (19), 2210-2211

CODEN: CHCOFS; ISSN: 1359-7345

PB Royal Society of Chemistry

DT Journal

LA English

CC 52-3 (Electrochemical, Radiational, and Thermal Energy Technology) Section cross-reference(s): 78

AB Metal imides (Li₂NH, CaNH), a metal amide (LiNH₂) and metal hydrides (LiH, CaH₂) were synthesized by ball milling of their resp. metal nitrides (Li₃N, Ca₃N₂) in a H₂ atmosphere at 1 MPa at room temperature

ST **hydrogen storage** metal nitride mechanochem reaction ball milling

IT Mechanochemical reaction

(**hydrogen storage** by metal nitrides through mechanochem. reactions)

IT Nitrides

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); **PROC (Process)**

(**hydrogen storage** by metal nitrides through mechanochem. reactions)

IT **1333-74-0, Hydrogen**, processes 12013-82-0, Calcium nitride (Ca₃N₂) 26134-62-3, Lithium nitride (Li₃N)

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); **PROC (Process)**

(**hydrogen storage** by metal nitrides through mechanochem. reactions)

IT **7580-67-8P**, Lithium hydride (LiH) **7782-89-0P**, Lithium amide (Li(NH₂)) **7789-78-8P**, Calcium hydride (CaH₂)

12135-01-2P, Lithium imide (Li₂(NH)) **12400-28-1P**, Calcium imide (Ca(NH))

RL: PNU (Preparation, unclassified); PREP (Preparation)

(**hydrogen storage** by metal nitrides through mechanochem. reactions)

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Ahn, C; Appl Phys Lett 1998, V73, P3378 HCAPLUS

(2) Amendola, S; J Power Sources 2000, V85, P186 HCAPLUS

- (3) Anon; Powder Diffraction File, International Center for Diffraction Data 2001
- (4) Balema, V; Chem Commun 2000, P1665 HCAPLUS
- (5) Balema, V; J Am Chem Soc 2002, V124, P6244 HCAPLUS
- (6) Bogdanovic, B; J Alloys Compd 1997, V253-254, P1 HCAPLUS
- (7) Bohger, J; J Mol Struct 1995, V348, P325 HCAPLUS
- (8) Chahine, R; Int J Hydrogen Energy 1994, V19, P161 HCAPLUS
- (9) Chambers, A; J Phys Chem B 1998, V102, P4253 HCAPLUS
- (10) Chen, P; Nature 2002, V420, P302 HCAPLUS
- (11) Dillon, A; Nature 1997, V386, P377 HCAPLUS
- (12) Ichikawa, T; J Alloys Compd 2004, V365, P271 HCAPLUS
- (13) Kojima, Y; Appl Phys Lett 2004, V84, P4113 HCAPLUS
- (14) Kojima, Y; Int J Hydrogen Energy 2002, V27, P1029 HCAPLUS
- (15) Newson, E; Int J Hydrogen Energy 1998, V23, P905 HCAPLUS
- (16) Tamura, T; J Alloys Compd 2002, V330-332, P522 HCAPLUS
- (17) Ye, Y; Appl Phys Lett 1999, V74, P2307 HCAPLUS

L50 ANSWER 7 OF 19 COMPENDEX COPYRIGHT 2005 EEI on STN
 AN 2004(45):10880 COMPENDEX
 TI Ternary **imides** for **hydrogen storage**.
 AU Xiong, Zhitao (Physics Department National University of Singapore, Singapore 117542, Singapore); Wu, Guotao; Hu, Jianjiang; Chen, Ping
 SO Advanced Materials v 16 n 17 Sep 3 2004 2004.p 1522-1525
 CODEN: ADVMEW ISSN: 0935-9648
 PY 2004
 DT Journal
 TC Experimental
 LA English
 AB The role of ternary Li-alkali earth metal **imides** for **hydrogen storage** was investigated. The ternary **imides** were synthesized by mixing, heating, hydrogenating and dehydrogenating lithium **amide** with corresponding **hydrides** of alkali earth metals. It was found that about 1.7 hydrogen atoms were adsorbed by one Li-Ca-N-H molecule, of which [similar to] 10% could be released at relatively high pressures. It was observed that **hydrogen storage** capacity, kinetics and thermodynamics of the lithium compounds changed with the chemical compositions. (Edited abstract) 15 Refs.
 CC 804.1 Organic Components; 694.4 Storage; 804.2 Inorganic Components; 641.1 Thermodynamics; 802.2 Chemical Reactions; 802.3 Chemical Operations
 CT *Organic compounds; X ray diffraction analysis; Pressure effects; Hydrogenation; Absorption; Synthesis (chemical); Temperature programmed desorption; Ternary systems; Hydrogen; Storage (materials); Lithium compounds; Nitrides; Thermodynamic properties
 ST **Hydrogen storage; Ternary imides;**
 Temperature programmed absorption (TPA); Pressure composition-isothermal (PCI) analysis
 ET Li; Ca*H*Li*N; Ca sy 4; sy 4; H sy 4; Li sy 4; N sy 4; Li-Ca-N-H

L50 ANSWER 8 OF 19 JICST-EPlus COPYRIGHT 2005 JST on STN
 AN 1040437365 JICST-EPlus
 TI **Hydrogen storage** by the use of reversible conversion between lithium **amide** and **imide**
 AU KUDO TOMOFUMI; SAKATA YOSHIHISA; IMAMURA HAYAO
 CS Yamaguchi Univ., Fac. Engineering, JPN
 SO Nippon Kagakkai Koen Yokoshu, (2004) vol. 84th, no. 1, pp. 363. Journal Code: S0493A (Fig. 2, Ref. 1)
 ISSN: 0285-7626
 CY Japan

DT Conference; Short Communication

LA Japanese

STA New

AB The decomposition and formation of lithium **amide** (LiNH_2) have been studied as an effective way to **store hydrogen** reversibly. To realize reversible **hydrogen storage** under mild conditions, nanosized lithium **amide** with high surface areas was prepared. The properties for **hydrogen storage** were evaluated by temperature programmed desorption, differential scanning calorimeter measurements, and ordinary volumetric techniques. (author abst.)

CC CD01010D; CB12043P (546; 544.723:53.06)

CT lithium compound; **amide**; **hydrogen storage**; sample preparation; reversible reaction; **imide**; activated carbon; thermal programmed desorption; X-ray diffraction

BT alkali metal compound; nitrogen compound; nitrogen group element compound; storage; preparation(material); chemical reaction; carbon material; inorganic material; material; thermodesorption; desorption; X-ray scattering; electromagnetic wave scattering; scattering; diffraction; coherent scattering

L50 ANSWER 9 OF 19 COMPENDEX COPYRIGHT 2005 EEI on STN

AN 2004(48):3199 COMPENDEX

TI Synthesis and dehydriding studies of mg-n-h systems.

AU Nakamori, Y. (Institute for Materials Research Tohoku University, Sendai 980-8577, Japan); Kitahara, G.; Orimo, S.

SO Journal of Power Sources v 138 n 1-2 Nov 15 2004 2004.p 309-312
CODEN: JPSODZ ISSN: 0378-7753

PY 2004

DT Journal

TC Theoretical; Experimental

LA English

AB Light-elemental **amides** and **imides** are recently regarded as potential candidates for high-performance **hydrogen storage** materials. In this studies, the single phases magnesium **amide** ($\text{Mg}(\text{NH}_2)_2$) and magnesium **imide** (MgNH) were successfully prepared by solid-gas reactions of MgH_2 with ammonia at 613 K and 653 K, respectively. Subsequently, $\text{Mg}(\text{NH}_2)_2$ was mixed with different molars of MgH_2 or LiH in order to systematically investigate the dehydriding properties. With increasing temperature, the mixtures of $\text{Mg}(\text{NH}_2)_2$ and MgH_2 desorb ammonia at approximately 630 K, similar to the decomposition reaction of $\text{Mg}(\text{NH}_2)_2$ alone. On the other hand, the mixture of $\text{Mg}(\text{NH}_2)_2$ and 4 M of LiH desorbs only hydrogen during heating because of the "ultra-fast" reaction of LiH with ammonia from $\text{Mg}(\text{NH}_2)_2$, unlike MgH_2 . \$CPY 2004 Elsevier B.V. All rights reserved. 24 Refs.

CC 542.2 Magnesium and Alloys; 549.2 Alkaline Earth Metals; 804.1 Organic Components; 804.2 Inorganic Components; 542.4 Lithium and Alloys; 549.1 Alkali Metals

CT *Magnesium printing plates; Synchrotron radiation; Hydrogen; Heating; Thermodynamics; X ray diffraction analysis; Gas chromatography; Amines; Ammonia; Lithium

ST **Hydrogen storage**; Solid-gas reaction; **Amide**;
Imide

ET $\text{H}^*\text{Mg}^*\text{N}$; ($\text{Mg}(\text{NH}$; Mg cp; cp; N cp; H cp; MgNH ; H^*Mg ; MgH ; $\text{Mg}(\text{NH}$; H^*Li ; LiH ; Li cp

L50 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:832248 HCAPLUS

ED Entered STN: 12 Oct 2004

TI (LiNH₂-MgH₂): a viable **hydrogen storage** system
 AU Luo, Weifang
 CS Analytical Material Science Department, MS 9403, Sandia National
 Laboratories, Livermore, CA, 94550, USA
 SO Journal of Alloys and Compounds (2004), 381(1-2), 284-287
 CODEN: JALCEU; ISSN: 0925-8388
 PB Elsevier B.V.
 DT Journal
 LA English
 CC 52-3 (Electrochemical, Radiational, and Thermal Energy Technology)
 AB One of the problems related to the employment of **hydrogen**-based
 fuel cells for vehicular transportation is on board storage.
Hydrogen storage in solids has long been recognized as
 one of the most practical approaches for this purpose. The capacity of
 existing storage materials is markedly below that needed for vehicular
 use. Recently Chen et al. (2002 and 2003) reported a lithium
 nitride/imide system, with a high capacity, 11.5%, however, its operating
 temperature and pressure are not satisfactory for vehicular application. In
 this research a new storage material was developed, which is from the
 partial substitution of lithium by magnesium in the nitride/imide system.
 The plateau pressure of this new Mg-substituted system is .apprx.30 bar
 and 200 °C with a H capacity of 4.5% and possibly higher. This is
 a very promising H-storage material for on board storage for vehicular
 applications.
 ST lithium magnesium amide imide hydride **hydrogen storage**
 dehydrogenation hydrogenation
 IT INDEXING IN PROGRESS
 IT Dehydrogenation
 Hydrogenation
 ((LiNH₂-MgH₂) as viable **hydrogen storage** system
 with reversible hydrogenation-dehydrogenation capacity)
 IT Pressure
 (effect on **hydrogen storage** capacity; (LiNH₂-MgH₂)
 as viable **hydrogen storage** system with reversible
 hydrogenation-dehydrogenation capacity)
 IT Fuel cells
 (hydrides, amides, and imides for **hydrogen storage**
 for; (LiNH₂-MgH₂) as viable **hydrogen storage** system
 with reversible hydrogenation-dehydrogenation capacity)
 IT **Storage**
 (of **hydrogen**; (LiNH₂-MgH₂) as viable **hydrogen**
storage system with reversible hydrogenation-dehydrogenation
 capacity)
 IT 12135-01-2, Lithium imide (Li₂(NH))
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM
 (Formation, nonpreparative); RACT (Reactant or reagent)
 ((LiNH₂-MgH₂) as viable **hydrogen storage** system
 with reversible hydrogenation-dehydrogenation capacity)
 IT 1333-74-0, **Hydrogen**
 RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation,
 nonpreparative); RACT (Reactant or reagent)
 ((LiNH₂-MgH₂) as viable **hydrogen storage** system
 with reversible hydrogenation-dehydrogenation capacity)
 IT 7782-89-0, Lithium amide (Li(NH₂))
 RL: PRP (Properties); RCT (Reactant); TEM (Technical or engineered
 material use); RACT (Reactant or reagent); USES (Uses)
 ((LiNH₂-MgH₂) as viable **hydrogen storage** system
 with reversible hydrogenation-dehydrogenation capacity)
 IT 7580-67-8, Lithium hydride (LiH)

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

((LiNH₂-MgH₂) as viable **hydrogen storage** system with reversible hydrogenation-dehydrogenation capacity)

IT **7693-27-8**, Magnesium hydride (MgH₂) 26134-62-3, Lithium nitride (Li₃N)

RL: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)

((LiNH₂-MgH₂) as viable **hydrogen storage** system with reversible hydrogenation-dehydrogenation capacity)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

- (1) Anon; CRC Handbook of Chemistry and Physics, 84th ed 2003-2004
- (2) Bogdanovic, B; J Alloys Compd 1997, V253-254, P1 HCAPLUS
- (3) Bogdanovic, B; J Alloys Compd 1999, V282, P84 HCAPLUS
- (4) Bogdanovic, B; J Alloys Compd 2000, V302, P36 HCAPLUS
- (5) Chen, P; J Phys Chem B 2003, V107, P10967 HCAPLUS
- (6) Chen, P; Nature 2002, V420(21), P302
- (7) Luo, W; J Less-Common Met 1988, V141, P103 HCAPLUS
- (8) Majzoub, E; J Alloys Compd 2003, V356-357, P363 HCAPLUS
- (9) Sandrock, G; J Alloys Compd 1999, V293-295, P877 HCAPLUS

L50 ANSWER 11 OF 19 COMPENDEX COPYRIGHT 2005 EEI on STN DUPLICATE 2

AN 2004(29):7204 COMPENDEX

TI **Hydrogen storage** properties of Li related and C related materials.

AU Ichikawa, Takayuki (Nat. Sci. Ctr. for Basic Res./Devt. Hiroshima University, Higashi-Hiroshima, 739-8521, Japan); Fujii, Hironobu

MT Advanced Materials for Energy Conversion II.

MO TMS, Reactive Metals Committee of the Light Metals Division; University of Nevada

ML Charlotte, NC., United States

MD 14 Mar 2004-18 Mar 2004

SO Advanced Materials for Energy Conversion II 2004.p 225-232
ISBN: 0873395743

PY 2004

MN 63270

DT Conference Article

TC Experimental

LA English

AB Hydrogenating and dehydrogenating properties of carbon-related and lithium-related materials as a candidate of **hydrogen storage** media were deeply investigated. As the carbon related materials, we examined hydrogen desorption properties of the hydrogenated nano-structured graphite prepared by ball milling under hydrogen atmosphere. The results obtained indicate that a small amount of iron contamination during milling process plays a quite important role as a catalyst for hydrogen absorption/desorption properties, leading a typical two-peak structure in the thermal desorption mass spectroscopy (TDMS) profile which is due to existence of highly dispersing iron on the nano-structured graphite. In the case of Li related materials, the 1:1 mixture of lithium **amide** (LiNH₂ and lithium **hydride** (LiH) containing a small amount of TiCl₃ or VCl₃ (1mol %) prepared by ball milling under H₂ gas atmosphere desorbed a large amount of hydrogen ([similar to]5.5 weight%) in the temperature range from 150 to 250deg C under the heating rate of 5 deg C/min and also showed an excellent cycle retention with an effective hydrogen capacity of more than 5 weight% until at least 3 cycles. In addition, the lithium-**imide** (Li₂NH) produced by hydrogen desorption of the above mixture indicated a quick hydrogen

absorption reaction even at 150deg C. 15 Refs.
 CC 804 Chemical Products Generally; 802.3 Chemical Operations; 542.4 Lithium and Alloys; 549.1 Alkali Metals; 482.2 Minerals; 933.1 Crystalline Solids
 CT *Carbon; Ball milling; Graphite; Nanostructured materials; Iron; Catalysts; Desorption; Hydrogen; Lithium
 ST Hydrogen desorption; **Hydrogen storage** media; Nano-structured graphite; Desorption peaks
 ET Li; H*Li*N; LiNH; Li cp; cp; N cp; H cp; H*Li; LiH; Cl*Ti; TiCl; Ti cp; Cl cp; Cl*V; VCl; V cp; H; Li2NH; C

L50 ANSWER 12 OF 19 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN

AN 2004-142812 [14] WPIX

DNN N2004-113877 DNC C2004-057415

TI **Hydrogen storage** method for **hydrogen** fuel cells by bringing hydrogen gas into contact with organic compound under pressure.

DC A85 E19 E36 J06 L03 X16

IN YAGI, M

PA (KURK) KURITA WATER IND LTD; (YAGI-I) YAGI M

CYC 104

PI WO 2004000857 A1 20031231 (200414)* JA 69 C07F009-50
 RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS
 LU MC MW MZ NL OA PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW
 W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
 DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
 KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NI NO NZ OM PH PL
 PT RO RU SC SD SE SG SK SL TJ TM TN TR TT TZ UA UG US UZ VC VN YU
 ZA ZM ZW

EP 1428831 A1 20040616 (200439) EN C07F009-50
 R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV
 MC MK NL PT RO SE SI SK TR

AU 2003242146 A1 20040106 (200447) C07F009-50

US 2004230084 A1 20041118 (200477) C07C009-00

ADT WO 2004000857 A1 WO 2003-JP7318 20030610; EP 1428831 A1 EP 2003-733334
 20030610, WO 2003-JP7318 20030610; AU 2003242146 A1 AU 2003-242146
 20030610; US 2004230084 A1 Cont of WO 2003-JP7318 20030610, US 2004-804108
 20040319

FDT EP 1428831 A1 Based on WO 2004000857; AU 2003242146 A1 Based on WO
 2004000857

PRAI JP 2003-24590 20030131; JP 2002-178755 20020619

IC ICM C07C009-00; C07F009-50

ICS C07C015-18; C07C015-27; C07C033-26; C07C033-28; C07C039-15;
 C07C039-17; C07C043-205; C07C057-22; C07C069-84; C07C233-09;
 C07C233-65; C07C275-00; C07D235-02; C07J009-00; C08B037-08;
 C08B037-16

AB WO2004000857 A UPAB: 20040226

NOVELTY - A method for **storing hydrogen** comprises bringing **hydrogen** gas into contact with an organic compound (A) under pressure.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:

(1) A hydrogen inclusion compound in which hydrogen is included in a host compound by contact reaction;

(2) Production of a hydrogen inclusion compound, comprising dissolving the host compound in a solvent, and passing hydrogen through the solution while recrystallizing the host compound and introducing hydrogen molecules into the crystal lattice; and

(3) Production of a hydrogen inclusion compound, comprising bringing hydrogen gas into contact with the host compound under pressure.

USE - For hydrogen fuel cells.

ADVANTAGE - The method gives stable **storage** of **hydrogen** with a relatively light weight in conditions close to ordinary temperature and pressure, while the **stored hydrogen** can be easily discharged, e.g., by heating.

Dwg.0/26

FS CPI EPI
FA AB; DCN
MC CPI: A12-E06; E31-A02; J06-B06; L03-E04F
EPI: X16-C

L50 ANSWER 13 OF 19 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2003-666681 [63] WPIX
DNN N2003-532052 DNC C2003-181776
TI Electrode for lithium secondary battery, contains active material mixture containing binder particles polydispersed into active material powder, provided on collector.
DC A85 L03 X16
PA (SAOL) SANYO ELECTRIC CO LTD
CYC 1
PI JP 2003109598 A 20030411 (200363)* 9 H01M004-62
ADT JP 2003109598 A JP 2001-302888 20010928
PRAI JP 2001-302888 20010928
IC ICM H01M004-62
ICS H01M004-02; H01M004-04; H01M004-58
ICA H01M010-40
AB JP2003109598 A UPAB: 20031001

NOVELTY - The electrode contains an active material mixture, provided on a collector. The active material mixture contains binder particles polydispersed into an active material powder.

DETAILED DESCRIPTION - An INDEPENDENT CLAIM is also included for manufacture of battery electrode.

USE - Used as electrodes such as hydrogen occlusion alloy electrode, nickel electrode and cadmium electrode of lithium secondary battery, nickel-**hydrogen storage** battery, and nickel-cadmium storage battery.

ADVANTAGE - The battery electrode has increased contact area of binder and active material, and excellent adhesion.

Dwg.0/0

FS CPI EPI
FA AB
MC CPI: A12-E06A; L03-E01B5B
EPI: X16-B01F1; X16-E01; X16-E08A; X16-E09

L50 ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:58220 HCAPLUS
DN 141:263271
ED Entered STN: 23 Jan 2004
TI Development of high capacity lithium based **hydrogen storage** materials
AU Ichikawa, Takayuki; Fujii, Horonobu
CS Dep. of Natural Science Research and Development Center, Hiroshima University, Japan
SO Kinzoku (2003), 73(11), 1110
CODEN: KNZKAI; ISSN: 0368-6337
PB Agune Gijutsu Senta
DT Journal
LA Japanese
CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)

Section cross-reference(s): 66

- AB The **hydrogen** release characteristics of LiNH₂-LiH system were investigated as a part of study on **hydrogen storage** materials. The H release characteristics is significantly improved in the presence of TiCl₃ catalyst.
- ST **hydrogen storage** material lithium imide hydride; lithium amide hydride system **hydrogen** release characteristics
- IT 7705-07-9, Titanium trichloride, uses
 RL: CAT (Catalyst use); USES (Uses)
 (**hydrogen** release catalyst for lithium amide-lithium hydride system)
- IT 7580-67-8, Lithium hydride 7782-89-0, Lithium amide 12135-01-2, Lithium imide
 RL: CPS (Chemical process); DEV (Device component use); PEP (Physical, engineering or chemical process); **PROC (Process)**; USES (Uses)
 (**hydrogen storage** material lithium imide-lithium hydride-lithium amide system system)
- IT 1333-74-0, **Hydrogen**, processes
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); **PROC (Process)**
 (lithium imide-lithium hydride-lithium amide system system for storage of)

L50 ANSWER 15 OF 19 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN

AN 2002-322147 [36] WPIX

DNN N2002-252572 DNC C2002-093785

TI Composite for containers, is formed by heat integration of fiber bundle consisting of textile fabric, knit fabric, nonwoven fabric, net-like object, honey-comb like object, and thermoplastic **polyamide** film.

DC A92 P73 Q25 Q69

PA (DUPO) DU PONT TORAY CO LTD; (FUJH) FUJI HEAVY IND LTD; (SAKA-N) SAKASE ADTECH CO

CYC 1

PI JP 2002019062 A 20020122 (200236)* 5 B32B027-34

ADT JP 2002019062 A JP 2000-208043 20000710

PRAI JP 2000-208043 20000710

IC ICM B32B027-34

ICS B32B005-02; B64D037-06; B64G001-40; C08J005-06; F17C003-00

ICI C08L079:08

AB JP2002019062 A UPAB: 20020610

NOVELTY - The composite is formed by heat integration of a thermoplastic **polyimide** film and a fiber bundle which consists of fiber, textile fabric, knit fabric, nonwoven fabric, net-like object and honey-comb like object.

DETAILED DESCRIPTION - An INDEPENDENT CLAIM is also included for the container.

USE - For containers (claimed) used for **storing** liquid oxygen, **hydrogen**, nitrogen and helium for aerospace relationships such as aircraft, satellite and airship.

ADVANTAGE - The light weight composite of excellent strength and low temperature characteristics, is obtained.

Dwg.0/0

FS CPI GMPI

FA AB

MC CPI: A05-J01B; A08-R01; A11-B09A1; A12-P01B

L50 ANSWER 16 OF 19 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN

AN 2002-114560 [15] WPIX

DNN N2002-085356 DNC C2002-035273
 TI Preparation of spherical or ellipsoidal pyrolyzed hard carbon material, useful e.g. as negative electrode material for secondary lithium batteries, **hydrogen storage** material, solid lubricant and adsorbent for toxic substances.
 DC E36 L03 X16
 IN CHEN, L; HUANG, X; LI, H; WANG, Q
 PA (PHYS-N) INST PHYSICS CHINESE ACAD SCI; (CHEN-I) CHEN L; (HUAN-I) HUANG X; (LIHH-I) LI H; (WANG-I) WANG Q
 CYC 23
 PI WO 2001098209 A1 20011227 (200215)* ZH 21 C01B031-02
 RW: AT BE CH CY DE DK ES FI FR GB GR IE IT LU MC NL PT SE TR
 W: CN JP US
 EP 1288160 A1 20030305 (200319) EN C01B031-02
 R: AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE TR
 CN 1422235 A 20030604 (200356) C01B031-02
 US 2003157014 A1 20030821 (200356) C01B031-00
 JP 2003535803 W 20031202 (200382) 26 C01B031-02
 ADT WO 2001098209 A1 WO 2001-CN613 20010424; EP 1288160 A1 EP 2001-935931 20010424, WO 2001-CN613 20010424; CN 1422235 A CN 2001-807830 20010424; US 2003157014 A1 WO 2001-CN613 20010424, US 2003-258350 20030306; JP 2003535803 W WO 2001-CN613 20010424, JP 2002-503655 20010424
 FDT EP 1288160 A1 Based on WO 2001098209; JP 2003535803 W Based on WO 2001098209
 PRAI CN 2000-106225 20000427
 IC ICM C01B031-00; C01B031-02
 AB WO 200198209 A UPAB: 20020306

NOVELTY - A pyrolyzed hard carbon material has spherical or ellipsoidal morphology with smooth surface, and has e.g. particle size of 0.05-100 micro m and coarseness of not more than 0.5% of the particle size, BET specific area of 1-4000 m²/g, inner pore size distribution between 0.3 and 50 nm, real density of 0.8-22 g/cm³, and tap density of 0.35-1.5 g/cm³, which contains not more than 10 weight% other elements.

DETAILED DESCRIPTION - A pyrolyzed hard carbon material has spherical or ellipsoidal morphology with smooth surface, and has particle size of 0.05-100 micro m and coarseness of not more than 0.5% of the particle size, BET specific area of 1-4000 m²/g, inner pore size distribution between 0.3 and 50 nm, d002 value by XRD method being 0.345-0.45 nm, values of Lc and La being 1-20 nm, real density of 0.8-22 g/cm³, and tap density of 0.35-1.5 g/cm³, which contains not more than 10 weight% other elements.

An INDEPENDENT CLAIM is also included for a process for preparing the material comprising:

(1) formulating a homogeneous dispersion system from a precursor of the synthetic hard carbon in a solvent at a concentration of 0.05-10 M, with the solvent including water, ethanol, acetone, **dimethylformamide** and other commonly-used organic solvents, while the precursor including glucose, sucrose, fructose, cellulose and starch as one type, and the other type being a mixture of phenol-formaldehyde resin, polyacrylonitrile, epoxide resin and solidifier of phthalic **anhydride** or a mixture of epoxide resin, polyformaldehyde and phenol, in which the precursor glucose, sucrose, cellulose or/and starch form a mixture with water as a homogeneous dispersion system at a 0.05-10 M, or a similarly formulated dispersion with the other precursors in the organic solvent(s) is applied particularly with not less than 25 weight% epoxide resin, or not less than 25 weight% phenol and the balance of polyformaldehyde in their mixtures;

(2) dewatering of the mixture in an autoclave at a filling degree of 30-95%, temperature rising until 150-300 deg. C at 30-600 deg. C/hr. then

maintaining at the temperature for 0-48 hrs. while stirring at 0-150 rpm;

(3) washing with water, ethanol or any of their mixtures after cooling rapidly at 1-3000 deg. C/hr. to room temperature, followed by filtration until the filtrate is clear for drying at 50-200 deg. C; and

(4) high-temperature carbonization under an inert atmosphere or hydrogen protection at flow-rate of 0.5-200 ml/min, or in vacuo at 1 multiply 10⁻³ mmHg to 380 mmHg with temperature rising at 30-300 deg. C/hr. until 600-3000 deg. C and at constant temperature for 0-48 hrs., then lowering temperature at 1-3000 deg. C/hr. quickly to room temperature.

USE - The prepared pyrolyzed hard carbon material is useful e.g. as negative electrode material for secondary lithium batteries, **hydrogen storage** material, solid lubricant, material for industrial-use electrical brushes and electrodes and alloy additives, and for producing high-tenacity composites, catalyst carriers, adsorbent for toxic substances and other special adsorbents, decolorants for food processing or materials for use in various organ substitutes (all claimed).

ADVANTAGE - Such material is easy to produce, with surface smoothness, regular appearance, even distribution of grain size and high stacking density.

DESCRIPTION OF DRAWING(S) - X-ray diffraction pattern of a spherical pyrolyzed hard carbon material made from sucrose as starting material. (Drawing includes non-English language text).

Dwg.2/3

FS CPI EPI
FA AB; GI; DCN
MC CPI: E11-S; E31-A02; E31-N03; L03-E01B3
EPI: X16-B01F1; X16-E01C

L50 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:319172 HCAPLUS

DN 131:107389

ED Entered STN: 25 May 1999

TI Theoretical study of ammonia activation by M⁺ (M=Sc, Ni, Cu)

AU Nakao, Yoshihide; Taketsugu, Tetsuya; Hirao, Kimihiko

CS Graduate School of Engineering, Department of Applied Chemistry, The University of Tokyo, Bunkyo-ku, Tokyo, 113, Japan

SO Journal of Chemical Physics (1999), 110(22), 10863-10873

CODEN: JCPSA6; ISSN: 0021-9606

PB American Institute of Physics

DT Journal

LA English

CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

Section cross-reference(s): 65

AB The reactions of the first-row transition metal cations, Sc⁺ (3D,1D), Ni⁺ (2D), Cu⁺ (1S), with NH₃ have been studied by the multiconfigurational and multireference-based theories, to clarify the similarities and differences in the reactivity of early (Sc⁺) and late (Ni⁺, Cu⁺) transition metal cations. In all the cases, the ion-dipole complex, MNH₃⁺, is initially formed with a C_{3v} symmetry structure, which is the most stable complex in the resp. potential energy surfaces except for Sc⁺ (1D). The M⁺-NH₃ binding energy was evaluated as 42.4, 37.8, 50.9, and 48.1 kcal/mol for Sc⁺ (3D), Sc⁺ (1D), Ni⁺, and Cu⁺, resp. In the second step, M⁺ is expected to activate one N-H bond of NH₃, leading to the insertion complex, HMNH₂⁺. In Sc⁺ (3D,1D), three different stationary points of HScNH₂⁺, i.e., Cs (in-plane), Cs (out-of-plane), and C_{2v} structures, were located, which correspond to a min. point, a first-order saddle point, and a second-order saddle point, resp. In these complexes, the singlet state

originating from Sc^+ (1D) is largely stabilized compared to the triplets. The singlet HScNH_2^+ (in-plane) is calculated to be the most stable compound. There are three dissociation channels from HScNH_2^+ , i.e., $\text{ScNH}_2^+ + \text{H}$, $\text{ScH}^+ + \text{NH}_2$, and $\text{ScNH}^+ + \text{H}_2$. The third dissociation occurs through the transition state of a four-centered structure, with a small activation barrier of 23 kcal/mol, in both singlet and triplet surfaces. As to the late transition metal cations Ni^+ and Cu^+ , there is no intermediate complex of HMNH_2^+ , thus, all the dissociations occur through highly vibrational excitations of MNH_3^+ . The calculated results are consistent with exptl. observations.

- ST scandium cation reaction ammonia binding energy transition state structure; nickel cation reaction ammonia binding energy transition state structure; copper cation reaction ammonia binding energy transition state structure; transition metal cation reaction ammonia
- IT Transition metals, reactions
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (ions; theor. study of ammonia activation by M^+ ($\text{M}=\text{Sc}, \text{Ni}, \text{Cu}$))
- IT Binding energy
 Ion-molecule reaction
 Ion-molecule reaction kinetics
 Transition state structure
 (theor. study of ammonia activation by M^+ ($\text{M}=\text{Sc}, \text{Ni}, \text{Cu}$))
- IT **1333-74-0, Hydrogen**, properties 12385-13-6, Atomic **hydrogen**, properties 13770-40-6, Amidogen **83018-00-2 115858-87-2 135789-74-1**
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); **PROC (Process)**
 (theor. study of ammonia activation by M^+ ($\text{M}=\text{Sc}, \text{Ni}, \text{Cu}$))
- IT 7664-41-7, Ammonia, reactions 14336-93-7, Scandium(1+), reactions 14903-34-5, Nickel(1+), reactions 17493-86-6, Copper(1+), reactions
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (theor. study of ammonia activation by M^+ ($\text{M}=\text{Sc}, \text{Ni}, \text{Cu}$))

RE.CNT 89 THERE ARE 89 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Abashkin, Y; J Phys Chem A 1997, V101, P8085 HCAPLUS
- (2) Ahlrichs, R; J Chem Phys 1985, V82, P890 HCAPLUS
- (3) Akinaga, Y; J Chem Phys 1997, V107, P415 HCAPLUS
- (4) Andersson, K; J Phys Chem 1990, V94, P5483 HCAPLUS
- (5) Armentrout, P; Metal-Ligand Interactions-Structure and Reactivity 1996, P23 HCAPLUS
- (6) Bakhtiar, R; J Am Chem Soc 1993, V115, P345 HCAPLUS
- (7) Becke, A; J Chem Phys 1992, V96, P2155 HCAPLUS
- (8) Becke, A; J Chem Phys 1993, V98, P5648 HCAPLUS
- (9) Blomberg, M; J Am Chem Soc 1991, V113, P424 HCAPLUS
- (10) Breckenridge, W; J Phys Chem 1996, V100, P14840 HCAPLUS
- (11) Chen, Q; Chem Phys Lett 1998, V284, P339 HCAPLUS
- (12) Chen, Q; J Phys Chem A 1998, V102, P3343 HCAPLUS
- (13) Chen, Y; J Am Chem Soc 1994, V116, P7815 HCAPLUS
- (14) Choe, Y; Chem Phys Lett 1998, V295, P380 HCAPLUS
- (15) Chong, D; J Chem Phys 1986, V84, P5606 HCAPLUS
- (16) Clemmer, D; J Am Chem Soc 1989, V111, P8280 HCAPLUS
- (17) Clemmer, D; J Phys Chem 1990, V94, P208 HCAPLUS
- (18) Clemmer, D; J Phys Chem 1990, V94, P3008 HCAPLUS
- (19) Clemmer, D; J Phys Chem 1991, V95, P3084 HCAPLUS
- (20) Davidson, E; J Comput Phys 1975, V17, P87
- (21) Dunning, T; J Chem Phys 1989, V90, P1007 HCAPLUS
- (22) Fisher, E; J Am Chem Soc 1992, V114, P2039 HCAPLUS

- (23) Frisch, M; GAUSSIAN 98, Revision A.5 1998
- (24) Goddard, W; Acc Chem Res 1973, V6, P368 HCAPLUS
- (25) Goebel, S; J Am Chem Soc 1995, V117, P6994 HCAPLUS
- (26) Gonzalez, C; J Chem Phys 1989, V90, P2154 HCAPLUS
- (27) Guo, B; J Phys Chem 1992, V96, P4879 HCAPLUS
- (28) Hanton, S; J Chem Phys 1992, V96, P5176 HCAPLUS
- (29) Hashimoto, T; J Chem Phys 1996, V104, P6244 HCAPLUS
- (30) Haynes, C; J Phys Chem 1995, V99, P6340 HCAPLUS
- (31) Haynes, C; J Phys Chem 1995, V99, P9110 HCAPLUS
- (32) Haynes, C; J Phys Chem 1996, V100, P111 HCAPLUS
- (33) Hendrickx, M; J Phys Chem A 1997, V101, P8540 HCAPLUS
- (34) Hirao, K; Chem Phys Lett 1992, V190, P374 HCAPLUS
- (35) Hirao, K; Chem Phys Lett 1992, V196, P397 HCAPLUS
- (36) Hirao, K; Chem Phys Lett 1993, V201, P59 HCAPLUS
- (37) Hirao, K; Int J Quantum Chem 1992, VS26, P517
- (38) Holthausen, M; J Phys Chem 1996, V100, P6236 HCAPLUS
- (39) Irigoras, A; J Phys Chem A 1998, V102, P293 HCAPLUS
- (40) Jahn, H; Proc R Soc London Ser A 1937, V161, P220
- (41) Johns, J; Can J Phys 1976, V54, P1804 HCAPLUS
- (42) Kapellos, S; J Phys Chem 1991, V95, P6860 HCAPLUS
- (43) Kawashima, Y; Chem Phys Lett 1997, V267, P82 HCAPLUS
- (44) Kickel, B; J Am Chem Soc 1995, V117, P764 HCAPLUS
- (45) Knowles, P; Chem Phys Lett 1985, V115, P259 HCAPLUS
- (46) Langhoff, S; J Phys Chem 1991, V95, P10677 HCAPLUS
- (47) Lee, C; Phys Rev B 1988, V37, P785 HCAPLUS
- (48) Lee, Y; J Phys Chem A 1997, V101, P9650 HCAPLUS
- (49) Luna, A; J Phys Chem A 1997, V101, P5931 HCAPLUS
- (50) Luna, A; J Phys Chem A 1998, V102, P4652 HCAPLUS
- (51) Mavridis, A; J Phys Chem 1991, V95, P6854 HCAPLUS
- (52) Meyer, F; J Am Chem Soc 1995, V117, P9740 HCAPLUS
- (53) Moore, C; Atomic Energy Levels; NSRD-NBS 1991, V3
- (54) Musaev, D; J Chem Phys 1994, V101, P10697 HCAPLUS
- (55) Musaev, D; J Phys Chem 1993, V97, P11435 HCAPLUS
- (56) Musaev, D; J Phys Chem 1996, V100, P11600 HCAPLUS
- (57) Nakano, H; Chem Phys Lett 1993, V207, P372 HCAPLUS
- (58) Nakano, H; J Chem Phys 1993, V99, P7983 HCAPLUS
- (59) Nakayama, K; Int J Quantum Chem 1997, V66, P157
- (60) Noll, R; J Phys Chem A 1998, V102, P386 HCAPLUS
- (61) Perry, J; J Phys Chem 1993, V97, P5238 HCAPLUS
- (62) Pettersson, L; J Chem Phys 1987, V87, P481 HCAPLUS
- (63) Roos, B; Chem Phys 1980, V48, P157 HCAPLUS
- (64) Roos, B; Int J Quantum Chem Symp 1980, V14, P175 HCAPLUS
- (65) Ryan, M; J Am Chem Soc 1995, V117, P2033 HCAPLUS
- (66) Schilling, J; J Am Chem Soc 1986, V108, P582 HCAPLUS
- (67) Schilling, J; J Phys Chem 1987, V91, P5616 HCAPLUS
- (68) Schmidt, M; J Comput Chem 1993, V14, P1347 HCAPLUS
- (69) Siegbahn, P; J Chem Phys 1984, V81, P1373 HCAPLUS
- (70) Siegbahn, P; Phys Scr 1980, V21, P323 HCAPLUS
- (71) Sievers, M; J Am Chem Soc 1998, V120, P1891 HCAPLUS
- (72) Stevens, W; Can J Chem 1992, V70, P612 HCAPLUS
- (73) Stevens, W; J Chem Phys 1984, V81, P6026
- (74) Sunderlin, L; J Am Chem Soc 1989, V111, P3845 HCAPLUS
- (75) Taketsugu, T; J Chem Phys 1996, V105, P1933 HCAPLUS
- (76) Taketsugu, T; J Chem Phys 1997, V106, P8504 HCAPLUS
- (77) Taketsugu, T; J Mol Struct: THEOCHEM 1998, V451, P163 HCAPLUS
- (78) Tilson, J; J Phys Chem 1991, V95, P5097 HCAPLUS
- (79) Tjelta, B; J Am Chem Soc 1995, V117, P5531 HCAPLUS
- (80) Truhlar, D; Science 1990, V249, P491 HCAPLUS
- (81) van Koppen, P; J Am Chem Soc 1991, V113, P2359 HCAPLUS

- (82) van Koppen, P; J Am Chem Soc 1994, V116, P3780 HCAPLUS
- (83) van Koppen, P; J Am Chem Soc 1998, V120, P5704 HCAPLUS
- (84) Walter, D; J Am Chem Soc 1998, V120, P3176 HCAPLUS
- (85) Werner, H; J Chem Phys 1985, V82, P5053 HCAPLUS
- (86) Werner, H; MOLPRO 1991
- (87) Wittborn, A; J Chem Phys 1997, V107, P4318 HCAPLUS
- (88) Yanai, T; J Chem Phys 1997, V107, P1137 HCAPLUS
- (89) Yi, S; J Phys Chem A 1998, V102, P395 HCAPLUS

L50 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:49677 HCAPLUS

DN 130:124717

ED Entered STN: 25 Jan 1999

TI Iron-mediated amination of hydrocarbons in the gas phase

AU Broenstrup, Mark; Kretzschmar, Ilona; Schroeder, Detlef; Schwarz, Helmut

CS Institut Organische Chemie, Technische Universitaet Berlin, Berlin,
D-10623, Germany

SO Helvetica Chimica Acta (1998), 81(12), 2348-2369

CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta AG

DT Journal

LA English

CC 22-4 (Physical Organic Chemistry)

Section cross-reference(s): 29, 67, 78

AB FeNH⁺ is chosen as a model system to probe the transition-metal-mediated transfer of imine groups in the gas phase by mass-spectrometric means. Ab initio calcns. at the MR-ACPF level predict FeNH⁺ to have a linear sextet ground state (6Σ⁺); a bent quartet state (4A'), and a linear doublet state (2Δ) are higher in energy by 0.14 eV and 0.51 eV, resp. The bond-dissociation energy is determined to D(Fe⁺-NH) = 69 ± 2 kcal mol⁻¹ using ion-mol. reactions. Charge-stripping expts. combined with ab initio calcns. yield an ionization energy of IE(FeNH⁺) = 15.7 ± 0.5 eV. The chemical behavior of FeNH⁺ towards O, water, H, aliphatic hydrocarbons,

benzene,

and toluene reveals an intrinsically high reactivity of FeNH⁺. Because a transfer of the NH fragment to the substrate is feasible in most cases, attractive amination reactions like CH₄ → methylamine, benzene → aniline, or toluene → benzylidenamine can be afforded by FeNH⁺.

ST iron imido mol electronic structure calcn; dissochn energy iron imido;
amination kinetics imidoiron org inorg substance

IT Amination kinetics

(amination reaction kinetics of FeNH⁺ with organic and inorg. substances)

IT Dissociation

(coulombic explosion; of FeNH₂⁺)

IT Amination

(enthalpy; of hydrocarbons with FeNH⁺)

IT Transition metal complexes

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(imides; FeNH⁺ as a model system to probe the transition-metal-mediated transfer of imine groups to hydrocarbons in the gas phase)

IT Bond energy

(iron-nitrogen bond energy of FeNH⁺; mol. and electronic structure, dissociation and ionization energy calculated for FeNH⁺ at MR-ACPF level)

IT Bond length

(iron-nitrogen bond length of FeNH⁺; mol. and electronic structure, dissociation and ionization energy calculated for FeNH⁺ at MR-ACPF level)

IT Electronic structure

(mol. and electronic structure, dissociation and ionization energy calculated for FeNH⁺ at MR-ACPF level)

IT Ionization potential
(of FeNH₂; formation and upper limit to ionization potential)

IT Molecular structure
(of FeNH⁺ and related species; mol. and electronic structure, dissociation and ionization energy calculated for FeNH⁺ at MR-ACPF level)

IT Bending vibration
Stretching vibration
(of FeNH⁺; mol. and electronic structure, dissociation and ionization energy calculated for FeNH⁺ at MR-ACPF level)

IT Electron density
(of FeNH₂⁺)

IT Free energy
(of FeO⁺ + NH₃ ion-mol. reaction; mol. and electronic structure, dissociation and ionization energy calculated for FeNH⁺ at MR-ACPF level)

IT Potential energy surface
(of electronic states of FeNH⁺; mol. and electronic structure, dissociation and ionization energy calculated for FeNH⁺ at MR-ACPF level)

IT Amination
(of hydrocarbons with FeNH⁺)

IT Hydrocarbons, reactions
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(of hydrocarbons with FeNH⁺)

IT Reaction enthalpy
(of ion-mol. reactions involving FeNH⁺)

IT Ion-molecule reaction
Ion-molecule reaction kinetics
(preparation and reactions of FeNH⁺)

IT Excited state
(quartet and doublet of FeNH⁺; mol. and electronic structure, dissociation and ionization energy calculated for FeNH⁺ at MR-ACPF level)

IT Ground state
(sextet of FeNH⁺; mol. and electronic structure, dissociation and ionization energy calculated for FeNH⁺ at MR-ACPF level)

IT 185148-36-1
RL: PRP (Properties)
(electron d.)

IT 74-85-1, Ethene, formation (nonpreparative) 109284-15-3 109801-95-8
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(formation in amination reaction of FeNH⁺ with C₂H₆)

IT 115-07-1, 1-Propene, formation (nonpreparative) 90823-21-5
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(formation in amination reaction of FeNH⁺ with C₃H₈)

IT 7664-41-7, Ammonia, reactions
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(formation in amination reaction of FeNH⁺ with H₂)

IT 7782-77-6, Nitrous acid 10102-43-9, Nitric oxide, formation (nonpreparative) 15092-05-4, Iron(1+), hydroxy-
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(formation in amination reaction of FeNH⁺ with O₂)

IT 62-53-3, Aniline, formation (nonpreparative) 74-90-8, Hydrocyanic acid, formation (nonpreparative) 34475-46-2, Aniline radical cation, formation (nonpreparative)
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(formation in amination reaction of FeNH⁺ with benzene)

IT 107-01-7, 2-Butene 102307-52-8
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (formation in amination reaction of FeNH+ with butane)

IT 127086-40-2 219908-12-0
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (formation in amination reaction of FeNH+ with isobutane)

IT 15600-68-7, Iron hydride (FeH) 109284-09-5 219908-13-1
 219908-19-7, Toluidine radical cation
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (formation in amination reaction of FeNH+ with toluene)

IT 72490-31-4, Iron imide (Fe(NH))
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
 (formation; formation and upper limit to ionization potential)

IT 74-89-5, Methylamine, formation (nonpreparative)
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (formation; formation by amination of methane with FeNH+)

IT 7439-89-6, Iron, formation (nonpreparative)
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (formation; formation in amination reaction of FeNH+ with benzene)

IT 7782-39-0, Deuterium, properties
 RL: PRP (Properties)
 (isotope effect; in FeNH+ + H2 reaction)

IT 14067-02-8, Iron1+, reactions
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
 (mol. and electronic structure calcn. at MR-ACPF level for)

IT 13774-92-0, Imidogen 15438-31-0, Iron2+, properties 19067-62-0, Aminyliumyl 219908-11-9
 RL: PRP (Properties)
 (mol. and electronic structure calcn. at MR-ACPF level for)

IT 115858-95-2, Iron(1+), imido-
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
 (mol. and electronic structure, dissociation and ionization energy calculated
 for FeNH+ at MR-ACPF level and amination reaction kinetics with organic and inorg. substrates)

IT 12434-84-3, Iron oxide ion (FeO+)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant; reaction with ammonia)

IT 7782-79-8, Hydrazoic acid 7803-49-8, Hydroxylamine, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant; reaction with iron cation)

IT 7732-18-5, Water, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant; reaction with iron imide cation)

IT 71-43-2, Benzene, reactions 74-82-8, Methane, reactions 74-84-0, Ethane, reactions 74-98-6, Propane, reactions 75-28-5, Isobutane 106-97-8, Butane, reactions 108-88-3, Toluene, reactions 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (reaction kinetics with FeNH+)

RE.CNT 105 THERE ARE 105 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE
 (1) Anhaus, J; J Am Chem Soc 1990, V112, P1642 HCAPLUS

- (2) Anon; Gmelin Handbook of Inorganic and Organometallic Chemistry Nitrogen Supplement B1 8th edn 1993
- (3) Anon; Houben-Weyl, Methoden der organischen Chemie 1957, V11
- (4) Anon; MOLPRO 96
- (5) Anon; Organometallic Ion Chemistry 1996
- (6) Arndtsen, B; J Am Chem Soc 1991, V113, P4871 HCAPLUS
- (7) Arndtsen, B; Organometallics 1993, V12, P2440 HCAPLUS
- (8) Babinec, S; J Am Chem Soc 1984, V10, P7718
- (9) Baranov, V; J Am Chem Soc 1995, V117, P12801 HCAPLUS
- (10) Becke, A; J Chem Phys 1993, V98, P5648 HCAPLUS
- (11) Becker, H; J Am Chem Soc 1994, V116, P1096 HCAPLUS
- (12) Bouchoux, G; Int J Mass Spectrom Ion Processes 1996, V153, P37 HCAPLUS
- (13) Bronstrup, M; unpublished results
- (14) Buckner, S; J Am Chem Soc 1988, V110, P6606 HCAPLUS
- (15) Buckner, S; Polyhedron 1988, V7, P1583 HCAPLUS
- (16) Clemmer, D; J Phys Chem 1990, V94, P208 HCAPLUS
- (17) Clemmer, D; J Phys Chem 1990, V94, P3008 HCAPLUS
- (18) Clemmer, D; J Phys Chem 1991, V95, P3084 HCAPLUS
- (19) Cummins, C; J Am Chem Soc 1988, V110, P8731 HCAPLUS
- (20) Cundari, T; J Am Chem Soc 1992, V114, P7879 HCAPLUS
- (21) Dai, P; Int J Mass Spectrom Ion Processes 1995, V144, P67 HCAPLUS
- (22) Du Bois, J; Acc Chem Res 1997, V30, P364 HCAPLUS
- (23) Eller, K; Inorg Chem 1990, V29, P3250 HCAPLUS
- (24) Eller, K; Int J Mass Spectrom Ion Processes 1989, V93, P243 HCAPLUS
- (25) Eller, K; J Am Chem Soc 1990, V112, P621 HCAPLUS
- (26) Fiedler, A; Chem Phys Lett 1993, V211, P242 HCAPLUS
- (27) Fiedler, A; Chem Phys Lett 1997, V271, P143 HCAPLUS
- (28) Fiedler, A; J Am Chem Soc 1994, V116, P10734 HCAPLUS
- (29) Filatov, M; J Phys Chem A 1998, V102, P3835 HCAPLUS
- (30) Forbes, R; Int J Mass Spectrom Ion Processes 1988, V83, P23 HCAPLUS
- (31) Frisch, M; Gaussian 94, Revision E.1 1995
- (32) Gibson, V; J Chem Soc Dalton Trans 1996, P4197 HCAPLUS
- (33) Glueck, D; J Am Chem Soc 1991, V113, P2041 HCAPLUS
- (34) Goldberg, N; Acc Chem Res 1994, V27, P347 HCAPLUS
- (35) Gountchev, T; J Am Chem Soc 1997, V119, P12831 HCAPLUS
- (36) Groves, J; J Am Chem Soc 1983, V105, P2073 HCAPLUS
- (37) Hartwig, J; Angew Chem 1998, V110, P2154
- (38) Hartwig, J; Angew Chem Int Ed Engl 1998, V37, P2046 HCAPLUS
- (39) Harvey, J; Chem Eur J 1996, V2, P1230 HCAPLUS
- (40) Hettich, R; J Am Chem Soc 1986, V108, P5086 HCAPLUS
- (41) Hori, K; J Am Chem Soc 1998, V120, P7651 HCAPLUS
- (42) Irikura, K; J Am Chem Soc 1989, V111, P75 HCAPLUS
- (43) Jorgensen, K; Inorg Chem 1993, V32, P1521
- (44) Kappes, M; J Am Chem Soc 1981, V103, P1286 HCAPLUS
- (45) Karrass, S; J Am Chem Soc 1989, V111, P9018 HCAPLUS
- (46) Karrass, S; Organometallics 1993, V12, P1449 HCAPLUS
- (47) Lammertsma, K; Angew Chem Int Ed Engl 1989, V28, P1321
- (48) Larock, R; Comprehensive Organic Transformations 1989
- (49) Lau, T; Inorg Chem 1996, V35, P2169 HCAPLUS
- (50) Lias, S; J Phys Chem Ref Data 1988, V17, P695
- (51) Loh, S; J Phys Chem 1989, V93, P3159 HCAPLUS
- (52) Maata, E; Inorg Chem 1979, V18, P2409
- (53) Marshall, A; Mass Spectrom Rev 1998, V17, P1 HCAPLUS
- (54) McCullough-Catalano, S; J Am Chem Soc 1993, V115, P1441 HCAPLUS
- (55) McKee, M; J Am Chem Soc 1990, V112, P2601 HCAPLUS
- (56) Moore, C; Atomic Energy Levels 1949
- (57) Musaev, D; J Chem Phys 1994, V101, P10697 HCAPLUS
- (58) Nugent, W; Inorg Chim Acta 1982, V65, PL91 HCAPLUS
- (59) Pavlov, M; J Phys Chem A 1997, V101, P1567 HCAPLUS

- (60) Ranatunga, D; Organometallics 1996, V15, P1242 HCAPLUS
- (61) Rocklage, S; J Am Chem Soc 1980, V102, P7808 HCAPLUS
- (62) Ryan, M; J Am Chem Soc 1994, V116, P9565 HCAPLUS
- (63) Schafer, D; J Am Chem Soc 1998, V120, P4881 HCAPLUS
- (64) Schaller, C; J Am Chem Soc 1996, V118, P591 HCAPLUS
- (65) Schalley, C; Chem Soc Rev 1998, V27, P91 HCAPLUS
- (66) Schnabel, P; J Phys Chem 1991, V95, P9688 HCAPLUS
- (67) Schofield, M; Inorg Chem 1991, V30, P3595 HCAPLUS
- (68) Schroder, D; Angew Chem 1990, V102, P1468
- (69) Schroder, D; Angew Chem Int Ed Engl 1990, V29, P1433
- (70) Schroder, D; Angew Chem, Int Ed Engl 1990, V29, P1431
- (71) Schroder, D; Angew Chem Int Ed Engl 1995, V34, P1973
- (72) Schroder, D; Helv Chim Acta 1992, V75, P1281
- (73) Schroder, D; Helv Chim Acta 1992, V75, P1792
- (74) Schroder, D; Inorg Chem 1994, V33, P5094
- (75) Schroder, D; Int J Mass Spectrom Ion Processes 1997, V161, P175
- (76) Schroder, D; J Am Chem Soc 1992, V114, P1215
- (77) Schroder, D; J Organomet Chem 1995, V504, P123
- (78) Schroder, D; J Phys Chem 1994, V98, P68
- (79) Schroder, D; J Phys Chem A 1998, V102, P3639
- (80) Schroder, D; Organometallics 1993, V12, P1972
- (81) Schroder, D; to be published in Angew Chem Int Ed Engl
- (82) Schultz, R; Organometallics 1992, V11, P828 HCAPLUS
- (83) Shaik, S; Chem Eur J 1998, V4, P193 HCAPLUS
- (84) Shaik, S; Helv Chim Acta 1995, V78, P1393 HCAPLUS
- (85) Srinivas, R; Int J Mass Spectrom Ion Processes 1991, V107, P369 HCAPLUS
- (86) Srinivas, R; J Am Chem Soc 1991, V113, P5970 HCAPLUS
- (87) Stephens, P; J Phys Chem 1994, V98, P11623 HCAPLUS
- (88) Steudel, R; Handbuch der preparativen anorganischen Chemie 1975, P455
- (89) Stockigt, D; Liebigs Ann Chem 1995, P429
- (90) Su, T; J Chem Phys 1982, V76, P5183 HCAPLUS
- (91) Su, T; J Chem Phys 1988, V89, P5355 HCAPLUS
- (92) Su, T; J Chem Phys 1994, V100, P4703 HCAPLUS
- (93) Turecek, F; Org Mass Spectrom 1992, V27, P1087 HCAPLUS
- (94) Walsh, P; J Am Chem Soc 1988, V110, P8729 HCAPLUS
- (95) Walsh, P; J Am Chem Soc 1992, V114, P1708 HCAPLUS
- (96) Walter, D; J Am Chem Soc 1998, V120, P3176 HCAPLUS
- (97) Werner, H; Theor Chim Acta 1990, V78, P175 HCAPLUS
- (98) Wesendrup, R; Angew Chem 1994, V106, P1232 HCAPLUS
- (99) Wesendrup, R; Angew Chem Int Ed Engl 1994, V33, P1174
- (100) Widmark, P; Theor Chim Acta 1990, V77, P291 HCAPLUS
- (101) Widmark, P; Theor Chim Acta 1991, V79, P419 HCAPLUS
- (102) Wullner, G; Chem Commun 1998, P1509 HCAPLUS
- (103) Yoshizawa, K; Chem Eur J 1997, V3, P1160 HCAPLUS
- (104) Yoshizawa, K; J Am Chem Soc 1998, V120, P564 HCAPLUS
- (105) Yoshizawa, K; Organometallics 1998, V17, P2825 HCAPLUS

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AN 1987-285996 [41] WPIX

DNC C1987-121246

TI **Storage**-stable low temperature-active **hydrogen** peroxide
bleach compsns. - comprise a liquid dispersion of a solid peracid precursor
peroxide activator in hydrogen peroxide solution.

DC D25 E14 P35

IN CARTY, D; MITCHELL, J D; ZIELSKE, A G

PA (CLR) CLOROX CO

CYC 16

PI EP 241137 A 19871014 (198741)* EN 13

R: BE CH DE ES FR GB GR IT LI LU NL SE

AU 8768033 A 19870917 (198744)
 JP 62230897 A 19871009 (198746)
 US 4772290 A 19880920 (198840) 9
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 EP 241137 B 19900718 (199029)
 R: BE CH DE ES FR GB GR IT LI LU NL SE
 DE 3763725 G 19900823 (199035)
 ES 2016840 B 19901201 (199102)
 ADT EP 241137 A EP 1987-302000 19870309; JP 62230897 A JP 1987-53204 19870310;
 US 4772290 A US 1986-838148 19860310
 PRAI US 1986-838148 19860310; US 1988-212831 19880629
 REP A3...8826; EP 92932; EP 94656; FR 2286912; No-SR.Pub
 IC A62D003-00; C01B015-00; C11D003-39; C11D007-54; C11D017-08; D06L003-02
 AB EP 241137 A UPAB: 19930922
 A liquid laundry bleach compsn comprises an acidic aq medium (pref pH 2-7) containing bleach-producing hydrogen peroxide (pref. 1-25 weight%) and a dispersed solid peracid precursor peroxide activator (pref 0.1-10 moles per mole peroxid). The activator is insoluble in the aqueous acid medium but soluble in alkaline laundry water.
 Opt the compsn also contains surfactants and fabric softener.
 A method of low temp bleaching of stains or soils from fabric is claimed.
 This has one or more base-ionisable solubiliser gps and is pref of formula (I) R=1-20C organic residue; and LG=aryloxy leaving gp; where at least one of R and LG has a covalently attached solubilising gp selected from aromatic and aliphatic acids and thioacids and their alkali(ne earth) metal salts, aromatic alcohols, thiols and **anhydrides, maleimides and sulphamides.**
 ADVANTAGE - The compsn combines the properties of being shelf-stable while being active at low temps. The activator is 10, 50 or 100 times more soluble at the bleaching pH than at the liquid compsn pH.
 0/0
 FS CPI GMPI
 FA AB
 MC CPI: D11-A01A1; D11-A01A2; D11-B01B; E06-A02A; E07-D02; E10-A08; E10-C01; E10-C02C; E10-C03; E10-C04; E10-E01; E10-E02D2; E10-E02F

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